

# Paul Mackenzie at Fermilab

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Andreas S. Kronfeld

**Fermilab** (6 September 1988– )

Lattice QCD at Fermilab:  
Celebrating the Career of Paul Mackenzie

Fermilab | 7–8 November 2019



# Paul's Professional Career

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- Ph. D., Cornell University, 1981
- Postdoc, Fermilab, 1981–1984
- Postdoc, Institute for Advanced Study, Princeton, 1984–1986
- Associate Scientist, Fermilab, 1986–1990
- Scientist I, II, III, Fermilab, 1990–2019 (Sci III → Distinguished Scientist)
- Distinguished Scientist Emeritus, [March 2019](#)–present

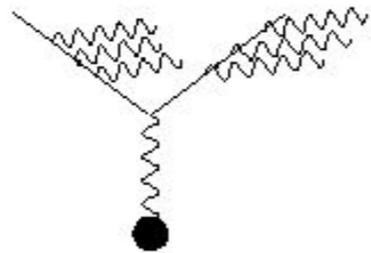
# Cornell

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Hideki Yukawa

Yukawa couplings



Donald Yennie

IR gauge bosons



Stan Brodsky

hadrons & QCD



Peter Lepage

perturbative &  
lattice QCD

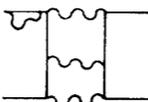
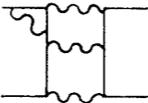
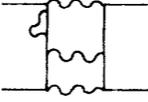
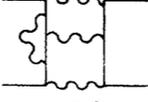
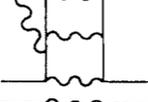
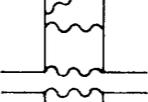
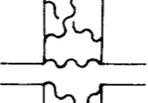
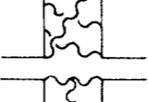
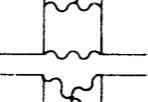
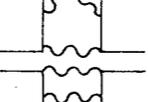
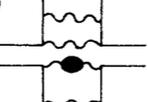
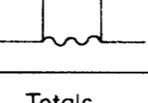


Paul Mackenzie

lattice QCD for  
Yukawa couplings

- Autumn 1980 at Cornell; Newman Lab; everyone is named Paul
- Espresso and cigarettes
- Summer 1981: birth of Rachel; Ph. D. on Upsilon decay to gluons

# Mackenzie and Lepage, PRL (1981)

| Sample Graph   | Number of Graphs in Class | Coefficient of $\alpha_s / \pi$ |                        |  |
|--|---------------------------|---------------------------------|------------------------|--|
|  |                           | Finite Piece                    | Ultraviolet Divergence | Infrared Divergence                    |
| a)    | 24                        | -3.591                          | $-\frac{2}{3} P$       | $-\frac{4}{3} \ln^2 \lambda^2 / m_b^2$ |
| b)    | 24                        | $-0.726 \pm .002$               | $-\frac{1}{6} P$       |  |
| c)    | 24                        | $-0.802 \pm .002$               | $-\frac{4}{3} P$       |  |
| d)    | 12                        | $-0.143 \pm .001$               | $-\frac{1}{12} P$      |  |
| e)    | 24                        | $.594 \pm .002$                 |                        |  |
| f)    | 12                        | $-10.424 \pm .022$              |                        | $\frac{4}{3} \ln^2 \lambda^2 / m_b^2$  |
| g)   | 24                        | $3.73 \pm .26$                  | $\frac{9}{2} P$        |  |
| h)  | 12                        | $9.76 \pm .22$                  | $\frac{9}{4} P$        |  |
| i)  | 24                        | 0.0                             |                        |  |
| j)  | 12                        | $-9.95 \pm .30$                 |                        |  |
| k)  | 18                        | $10.59 \pm .26$                 |                        |  |
| l)  | 9                         | $-3.02 \pm .04$                 |                        |  |
| m)  | 24                        | $-0.19 \pm .04$                 |                        |  |
| n)  | 72                        | $7.96 \pm .02$                  | $\frac{7}{4} P$        |  |
| Totals   | 315                       | $3.79 \pm .53$                  | $\frac{25}{4} P$       | 0                                      |

# Fermilab as postdoc

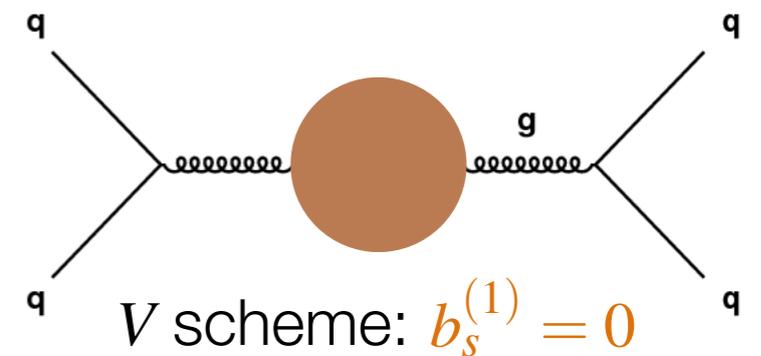
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- Famous "BLM" paper (1983)—academic grandfather, father, and son.
- In perturbative QCD, is there a guide to choosing the scale for  $\alpha_s(\mu)$ ?

$$\begin{aligned}\alpha_s(\mu)c^{(1)} &= \alpha_s(\mu) \int d^4q f(q) = \int d^4q \alpha_s(q) f(q) \\ &= \int d^4q \left\{ \alpha_s(q^*) + \alpha_s(q^*)^2 2\beta_0 \left[ \ln(q^*/q) - b_s^{(1)} \right] \right\} f(q) \\ &= \alpha_s(q^*) \int d^4q f(q)\end{aligned}$$

$\Rightarrow$

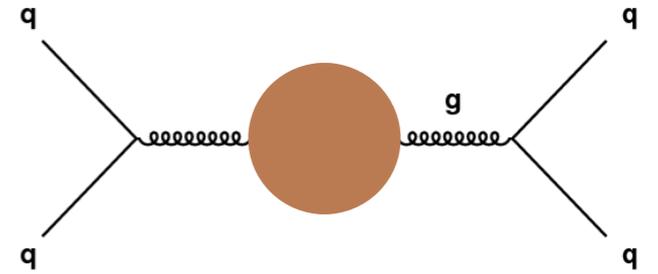
$$\ln(q^*) = \frac{1}{c^{(1)}} \int d^4q \ln(q) f(q) + b_s^{(1)}$$



- The BLM scale, as I learned it from Paul and Peter.

# Remarks

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- Stan Brodsky:
  - logarithm from inserting a massless quark loop on the gluon;
  - so, if the next order is available, you can find the logarithm from the  $n_f$ -dependent part;
  - package  $n_f$  into  $\beta_0$ , and choose  $q^*$  to remove the  $\beta_0$  part.
- George Sterman:
  - What makes BLM unique [among scale-setting prescriptions] is that it reaches out to higher order. It knows about Feynman diagrams.
- Also very useful in lattice perturbation theory [[Lepage, Mackenzie \(1993\)](#)].

# Pivot to Lattice QCD



- Early (if not first) calculation of a hadronic coupling [[Gottlieb, Mackenzie, Thacker, Weingarten \(1984\)](#)]:

$$g_{\rho\pi\pi} = \begin{array}{ll} 3.0 \pm 1.0_{\text{stat}} & \text{lattice QCD in the valence approximation} \\ 6.11 \pm 0.11 & \text{experimental measurement} \end{array}$$

Paul is always reminiscing, "back in the early days when we could get things right at the factor-of-two level."

- First calculation of the  $H$ -dibaryon mass [[Mackenzie, Thacker \(1985\)](#)]:
  - $H = \Lambda\Lambda = udsuds$ : is it stable or not? Cf. deuteron 2.2 MeV.
  - Hank and Paul found "no" in quenched (same as valence) approx.
  - Still not resolved; see, e.g., [arXiv:1805.03966](#).

# Pivot to Lattice QCD



- The difficulty in computing the binding energy of the  $H$  does not reflect a lack of care or effort.

Like the deuteron, it is evidence that the binding of nucleons into nuclei is subtle.

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Anecdotes, 1983–1988

# Outline

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- Fermilab take two: 1986–present
  - ACPMAPS
  - Fundamental parameters of QCD:  $\alpha_s(\mu)$  and quark masses
  - Massive fermions in lattice gauge theory
  - Cabibbo-Kobayashi-Maskawa matrix  Hashimoto, Friday, 4:00 PM
  - USQCD  Sugar, Thursday, 4:00 PM
  - Lattice QCD works!
  - Quark masses and CKM revisited  Gottlieb, Friday, 3:00 PM

SM Yukawa  
couplings

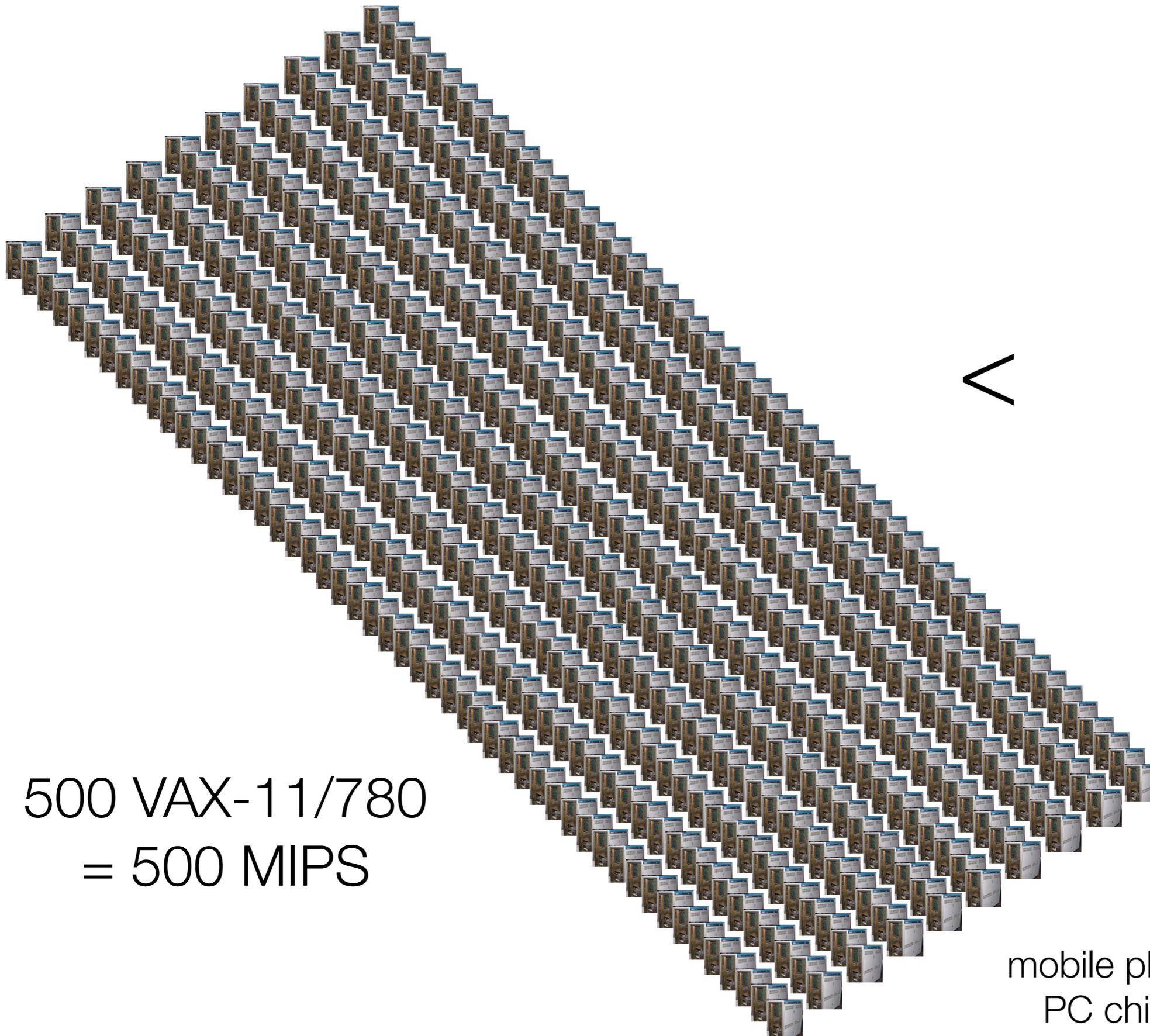
ACPMAPS



VAX-11/780

1 MIPS

fridge-sized



500 VAX-11/780  
= 500 MIPS



Latest  
mobile phones  $\leq$  10k MIPS  
PC chips  $\leq$  300k MIPS

# Lattice Gauge Theory as Computational Physics

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- In the mid-80s, it became clear that the available computing (e.g., VAX-11 780s for  $g_{Q\pi\pi}$  and  $M_H$ ) were not enough to meet aspirations.
- Build your own supercomputer from inexpensive parts. Some examples:
  - Norman Christ *et al.*,: "Columbia" (1985), QCDSF, QCDOC.
  - Don Weingarten *et al.* (IBM): GF-11.
  - N. Cabibbo *et al.* (APE Collaboration): APE, APE100, APEmille, ....
  - Tsukuba U.: QCDFPAX, CP-PACS, PACS-CS, HA-PACS, ....
- Influenced the transition in industry from big vector processors to parallel computers.

# ACPMAPS



- At Fermilab, Tom Nash was leading the Advanced Computer Program (ACP) to build cost-effective computing—mid-80s.
- Tom and Estia Eichten proposed ACPMAPS (ACP multi-array processor).



# Architecture

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- Floating point computations:
  - Gen 1: Floating-Point Array Processor (FPAP) used Weitek XL
  - Gen 2: D860 used (two/node) Intel i860 and a Xilinx field-programmable gate array—a lot fewer wires than the FPAP!
- Communications—crossbar switch BranchBus:
  - Bus-switch backplane (BSB).
  - Bus-switch interface board (BSIB).
- Balanced computer (similar computation and communication speeds).
- Complete computer (programmable in C, disk system, tape system).

# Canopy

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- Paul, with early input from Doug Toussaint, and then working with George Hockney, Mark Fischler, and Mike Uchima, laid down a gauntlet:
  - ACPMAPS should be easy for a "normal" theoretical physicist to program.
- Specify, document, and implement a library based on lattice concepts:
  - sites and links; grids (of sites and links); fields (on a grid);
  - lower levels of the software connected the physics to the machine;
  - independent RNG per site: same results for any number of nodes.
- When we needed a name, Hockney suggested `ydsfa`.

George Hockney,  
Don Husby, Tom Nash, Estia Eichten  
Bob Atac,  
Irwin Gaines, Mark Fischler, ASK  
(missing Paul, Joe Biel,  
Bill Haynes, Mike Uchima, others)



*Programmers and engineers in the Advanced Computer Program have designed both hardware and software for advanced parallel processing. The group has worked closely with a local electronics firm to develop the computing capability to perform a large number of independent tasks simultaneously, at a relatively low cost.*

among the first of a new genre of local-memory parallel processors, which have proven to be superb tools for solving many complex problems in science and engineering. When it was first used at Fermilab, the ACP made it possible to reconstruct the raw electronic data gathered in an experiment into a useful form in less than a quarter of the time it would have taken on all the Laboratory's other computers combined.

The first-generation ACP, which debuted in 1985, was substantially more cost-effective than any commercially available device, and national laboratories and universities

in Brazil, France, Switzerland, and the United States quickly placed orders.

Subsequent improvements combined new higher performance processors with more powerful and flexible software, called Cooperative Process Software. This software, together with "farms" of commercially available reduced-instruction-set computers, provides an inexpensive path to vast computational power. The Laboratory and Universities Research Association have licensed Omnibyte to produce and market a second-generation processor.

# Exabyte Anecdotes

no, not  $10^{18}$  bytes

# Exabyte Anecdotes



QCD

# ACPMAPS Computing

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- With ACPMAPS computations, we had two overarching aims:
  - learn how to study all sources of systematic uncertainties;
  - be relevant to experiment and phenomenology.
- We generated ensembles at three lattice spacings, approximately
  - 0.17 fm, 0.11 fm, 0.08 fm,
  - at a time when most lattice-QCD work used only one lattice spacing.
- The first is arguably very coarse, but it was computationally cheap:  
Could it be useful, and how?

# $\alpha_s$ (1992)



- Aida El-Khadra joined us as a postdoc, and we (Paul, Aida, George Hockney, and I) computed the charmonium spectrum.
- We didn't publish a paper on the charmonium spectrum per se.
- Instead, we published a determination of  $\alpha_s$ .
- Paul devised a way to correct for the quenched approximation, inspired by potential models:

$$\Lambda_{\overline{\text{MS}}}^{(0)} = 234 \text{ MeV} \Rightarrow \Lambda_{\overline{\text{MS}}}^{(4)} = 160_{-37}^{+47} \text{ MeV}$$

- Still gets good ratings from FLAG.

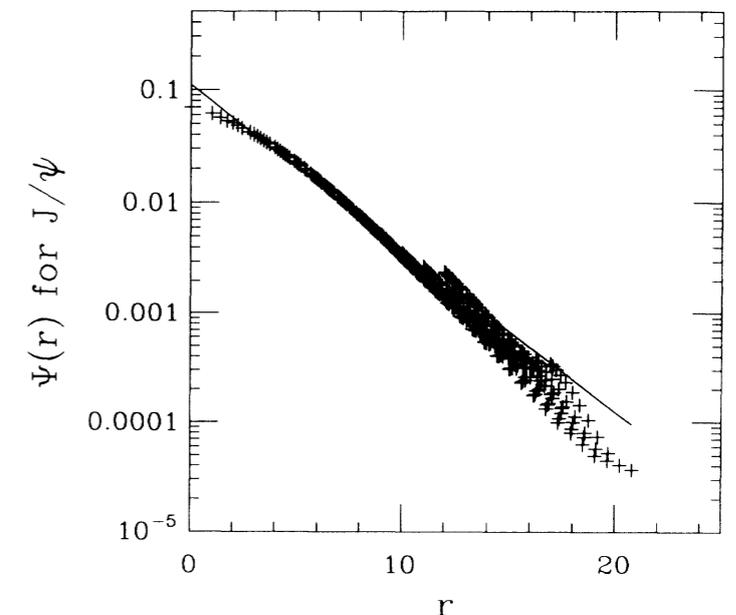


FIG. 1. The wave function of the  $\psi$  meson.

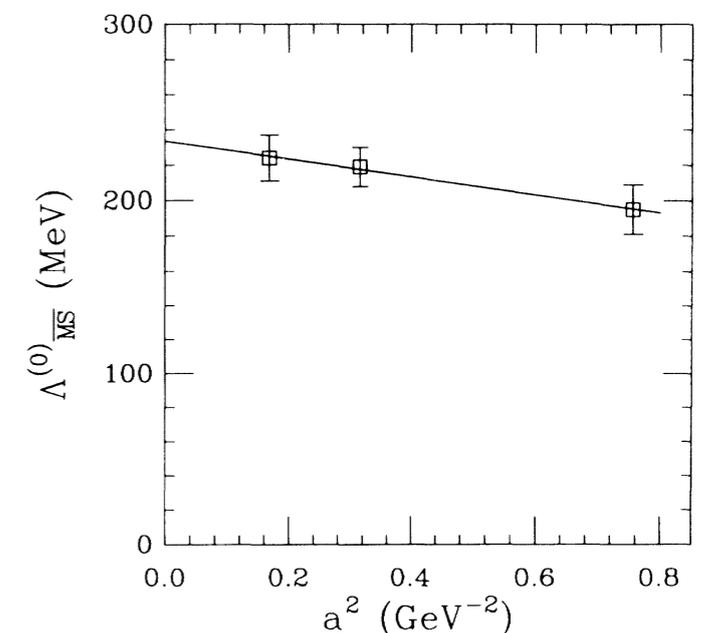


FIG. 2.  $\Lambda_{\overline{\text{MS}}}^{(0)}$  as a function of  $a^2$ .

# Light Quark Masses (1996)

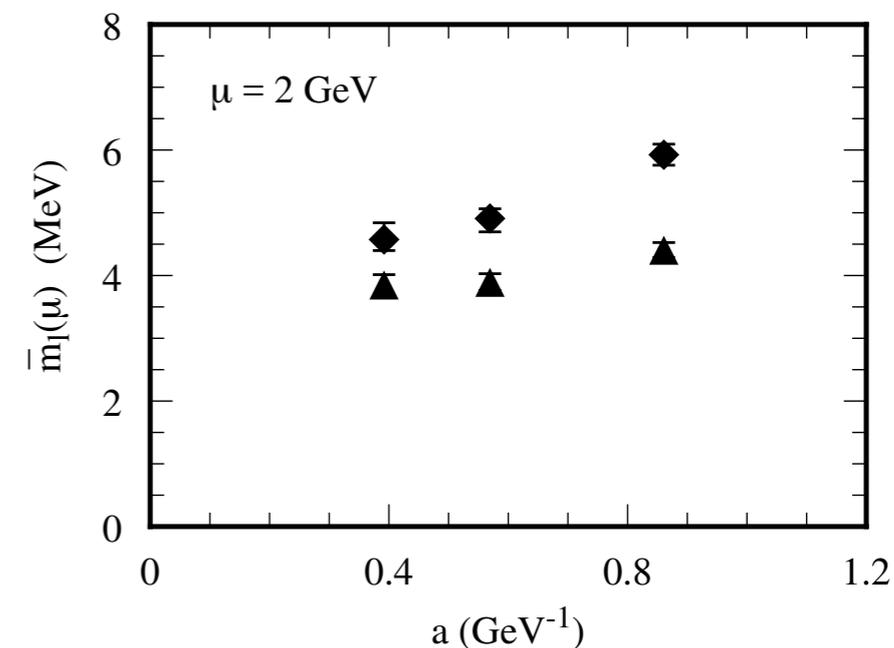
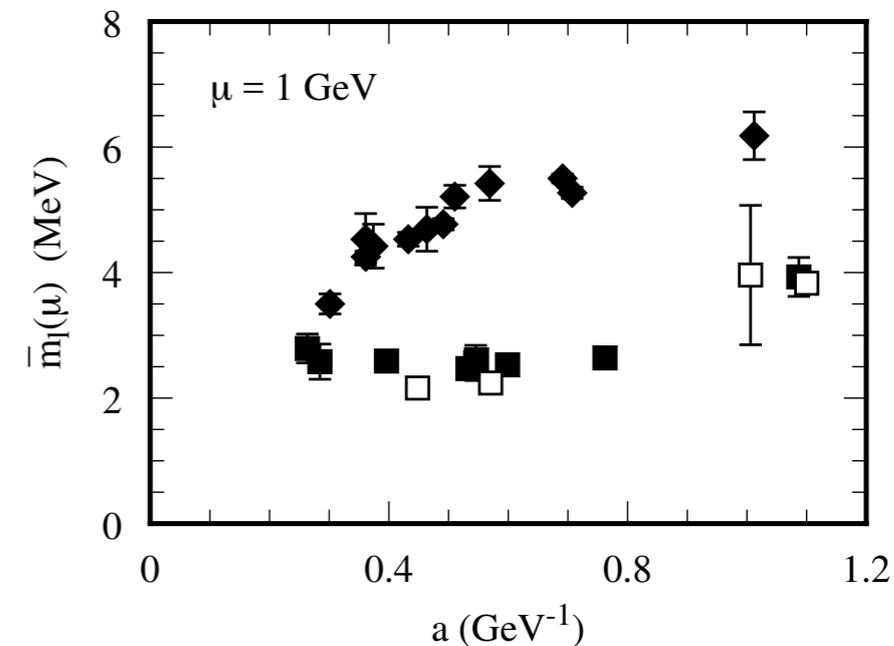


- Aida was now a professor. Brian Gough and Jim Simone were postdocs, and Tetsuya Onogi was visiting.
- My edits of the last PRL draft.
- The result was low compared to the conventional wisdom:

$$m_{s,\overline{\text{MS}}}(2 \text{ GeV}) = 95(16) \text{ MeV}$$

- Controversial then, but nowadays

$$m_{s,\overline{\text{MS}}}(2 \text{ GeV}) = \begin{cases} 94.49(79)_{\text{corr}}(63)_{\text{uncorr}} & \text{MeV} \\ 92.47(39)_{\text{stat}}(56)_{\alpha_s+\text{syst}} & \text{MeV} \\ 93.54(44)_{\text{corr}}(69)_{\text{uncorr}} & \text{MeV} \end{cases}$$



# The Fermilab Method

# Massive Fermions in Lattice Gauge Theory

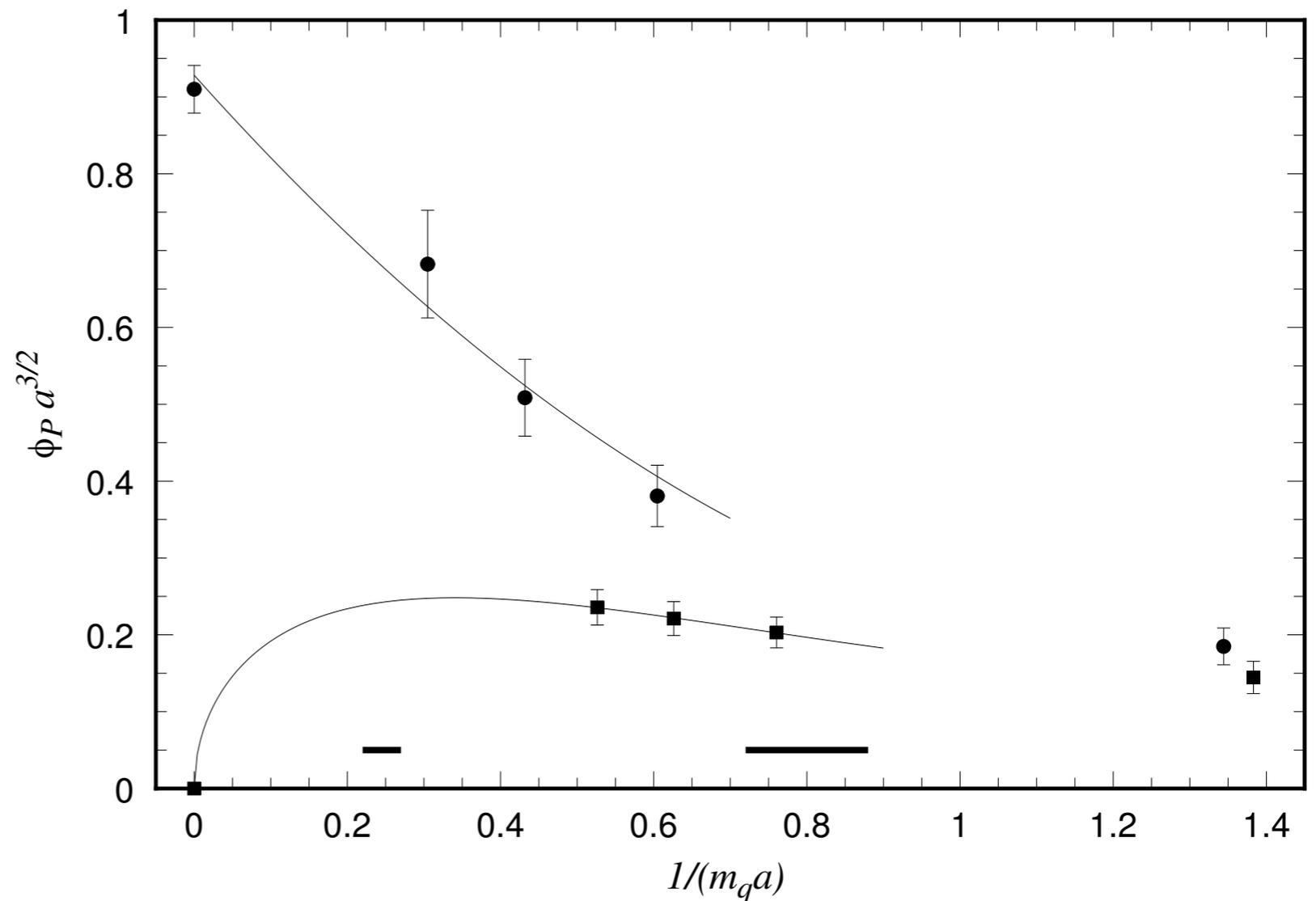
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- At Lattice 1987 in Seillac, Claude Bernard, Eichten, Guido Martinelli, and Lepage all (separately) emphasized the importance of heavy quarks.
- Eichten and Lepage pursued (slightly different) effective field theories:
  - HQET vs. NRQCD power counting, for heavy-light vs. quarkonium.
- Bernard and Martinelli pursued light-quark methods (Wilson fermions).
- Results for simple quantities (e.g., B-meson decay constants), which came out 1987–1991 did not agree—not even as well as they should in the primitive calculations of the day.
- Paul wanted to understand why, and started looking at variants of Wilson fermions.

# The Fermilab Method

- Three key ideas:
  - let the heavy quark hop differently in space & time;\*
  - reinterpret the pole mass of the quark (the kinetic mass);
  - normalize the field correctly.
- Often (then) erroneously called KLM.

El-Khadra, ASK, Paul [[hep-lat/9604004](https://arxiv.org/abs/hep-lat/9604004)]



\*keeping charge conjugation

CKM Matrix in the Late 1990s

# Full Error Budgets

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- Jim Simone now a staff member in Fermilab's Computing Division.
- Postdocs Shoji Hashimoto and Sinéad Ryan.
- $B$  and  $D$  meson decay constants in lattice QCD [[hep-ph/9711426](#)].
- Lattice QCD calculation of  $B \rightarrow D l \nu$  decay form-factors at zero recoil [[hep-ph/9906376](#)].
- Semileptonic decays  $B \rightarrow \pi l \nu$  and  $D \rightarrow \pi l \nu$  from lattice QCD [[hep-ph/0101023](#)].
- Lattice calculation of the zero-recoil form factor of  $B \rightarrow D^* l \nu$ : Toward a model-independent determination of  $|V_{cb}|$  [[hep-ph/0110253](#)].

# Full Error Budgets



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- Postdocs Shoji Hashimoto and Sinéad Ryan.
- $B$  and  $D$  meson decay constants in lattice QCD [[hep-ph/9711426](https://arxiv.org/abs/hep-ph/9711426)].

These four papers advanced the standard for estimating uncertainties in lattice QCD more than any comparable set of paper.

[[hep-ph/0101023](https://arxiv.org/abs/hep-ph/0101023)].

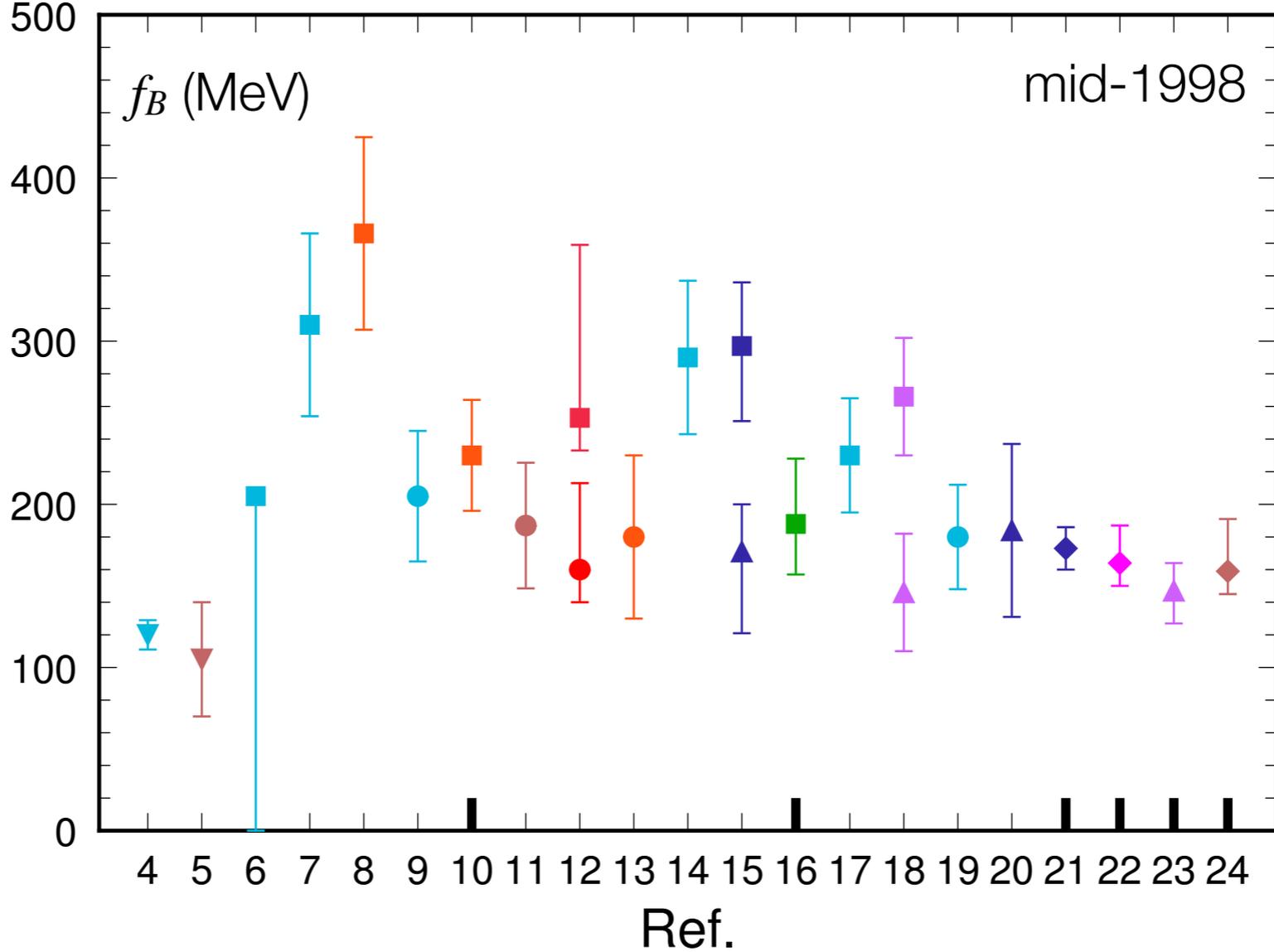
- Lattice calculation of the zero-recoil form factor of  $B \rightarrow D^* l \nu$ : Toward a model-independent determination of  $|V_{cb}|$  [[hep-ph/0110253](https://arxiv.org/abs/hep-ph/0110253)].

# Error Budgets for Pedagogy

TABLE IV. Budget of statistical and systematic uncertainties for  $h_{A_1}(1)$  and  $1 - h_{A_1}(1)$ . The row labeled “total systematic” does not include uncertainty from fitting, which is lumped with the statistical error. The statistical error is that after chiral extrapolation.

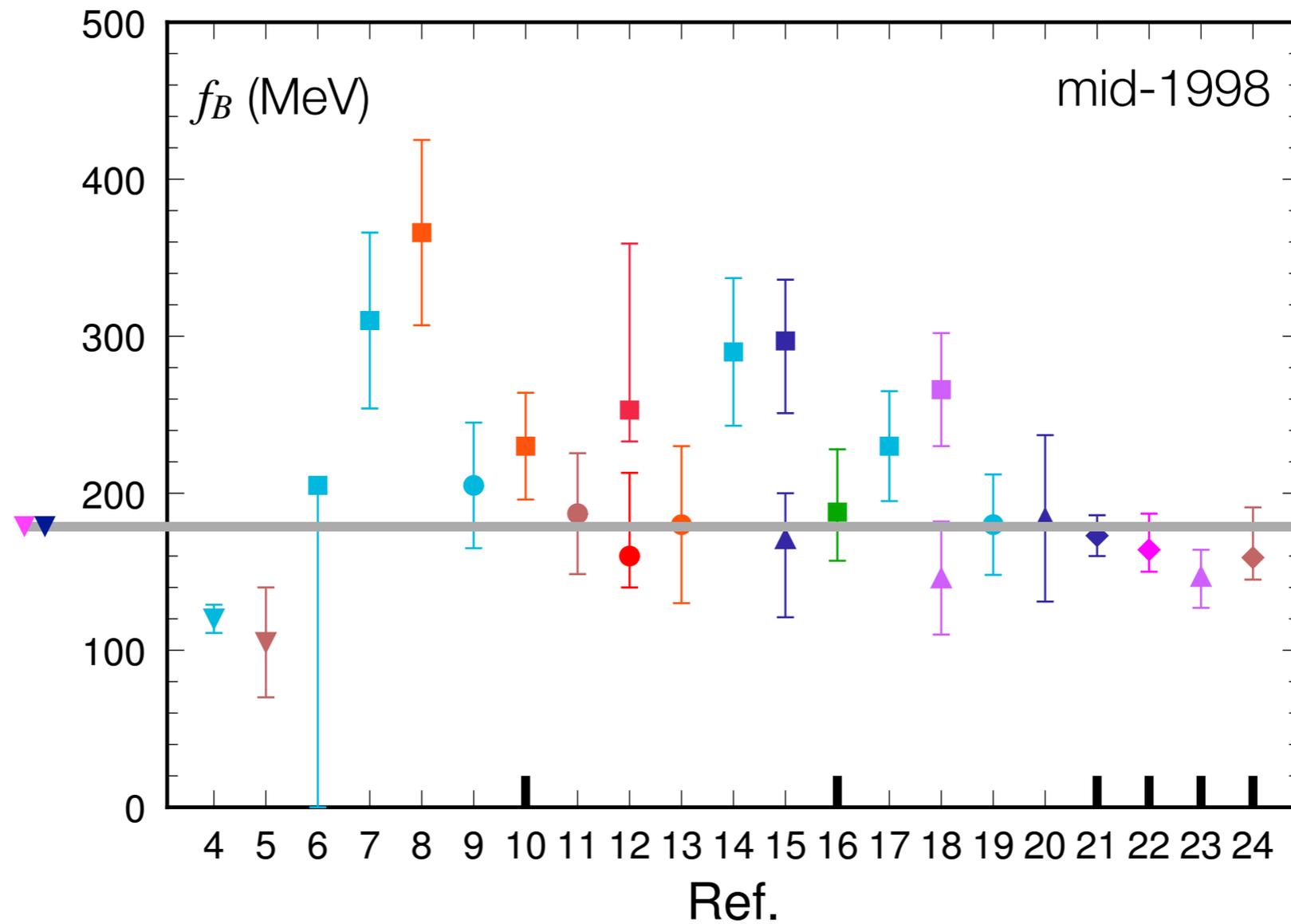
| uncertainty                      | $h_{A_1}$    |         | $1 - h_{A_1}$<br>(%) |          |
|----------------------------------|--------------|---------|----------------------|----------|
| statistics and fitting           | +0.0238      | -0.0173 | +27                  | -20      |
| adjusting $m_c$ and $m_b$        | +0.0066      | -0.0068 | + 8                  | - 8      |
| $\alpha_s^2$                     | $\pm 0.0082$ |         |                      | $\pm 9$  |
| $\alpha_s(\bar{\Lambda}/2m_Q)^2$ | $\pm 0.0114$ |         |                      | $\pm 13$ |
| $(\bar{\Lambda})^3/(2m_Q)^3$     | $\pm 0.0017$ |         |                      | $\pm 2$  |
| $a$ dependence                   | +0.0032      | -0.0141 | + 4                  | -16      |
| chiral                           | +0.0000      | -0.0163 | + 0                  | -19      |
| quenching                        | +0.0061      | -0.0143 | + 7                  | -16      |
| total systematic                 | +0.0171      | -0.0302 | +20                  | -35      |
| total (stat $\oplus$ syst)       | +0.0293      | -0.0349 | +34                  | -40      |

# And they fared quite well, despite quenching



# And they fared quite well, despite quenching

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USQCD

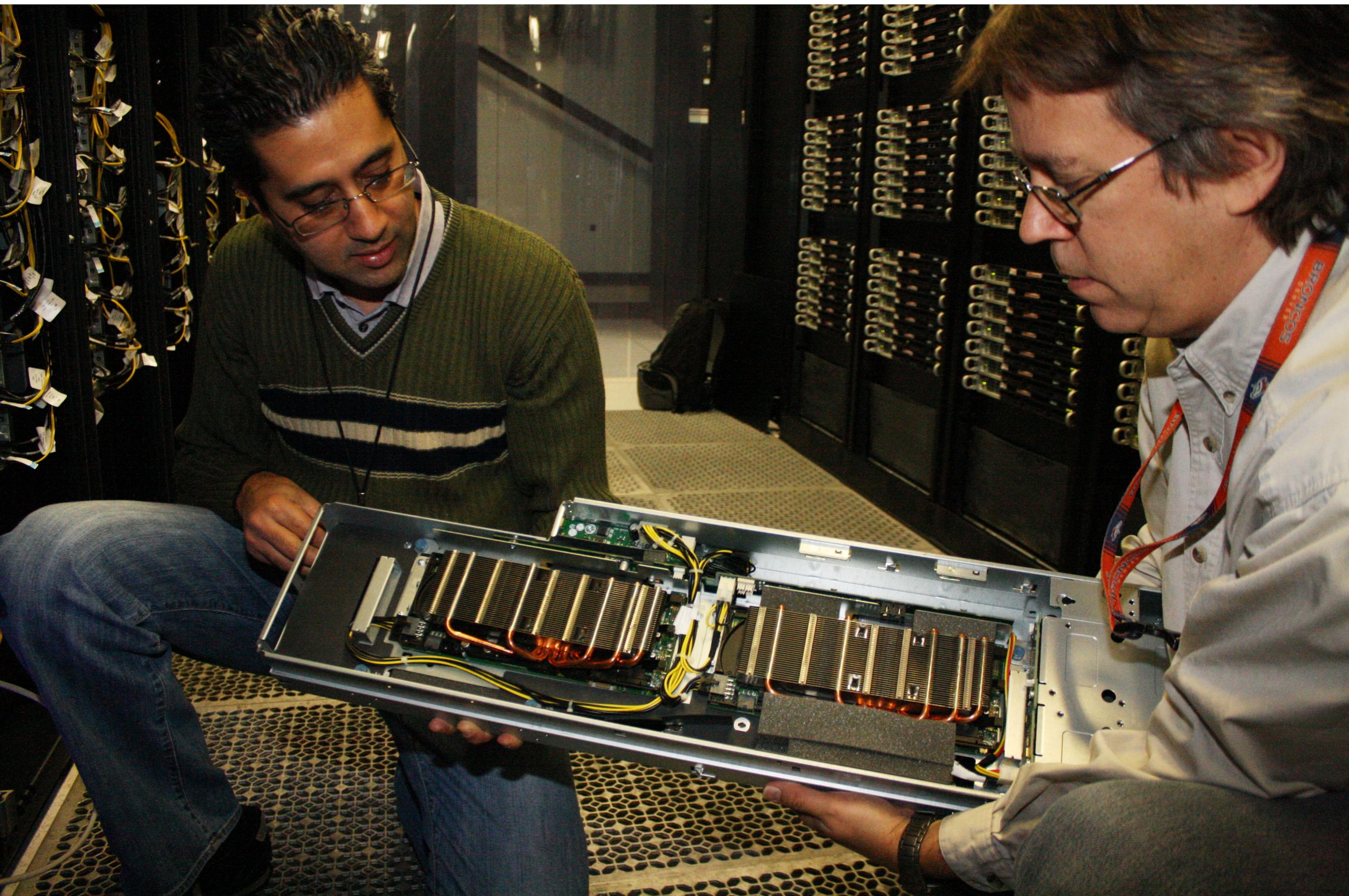
# USQCD Collaboration

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- A federation of science collaborations engaged in lattice gauge theory.
- Formation spurred by Jeff Mandula and Vicky White at (on loan to) DOE.
- Bob Sugar will give details.
- Here, how Paul's career evolved.
- Phase 1 (EC member): work with Don Holmgren on developing the PC-cluster model of lattice-QCD computing.
- Phase 2 (EC Chair and collaboration spokesman): physics at the bureaucracy frontier.



CPU cluster with Infiniband communication link



Amitoj Singh

GPU for lattice QCD

Don Holmgren

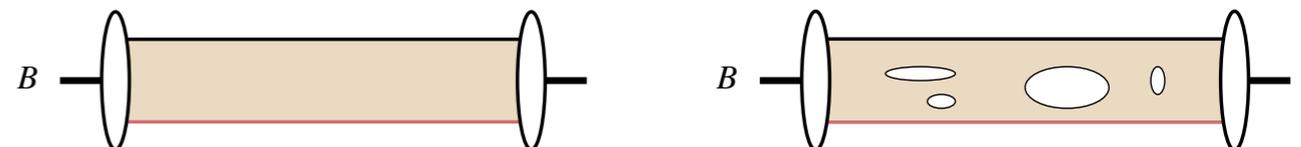
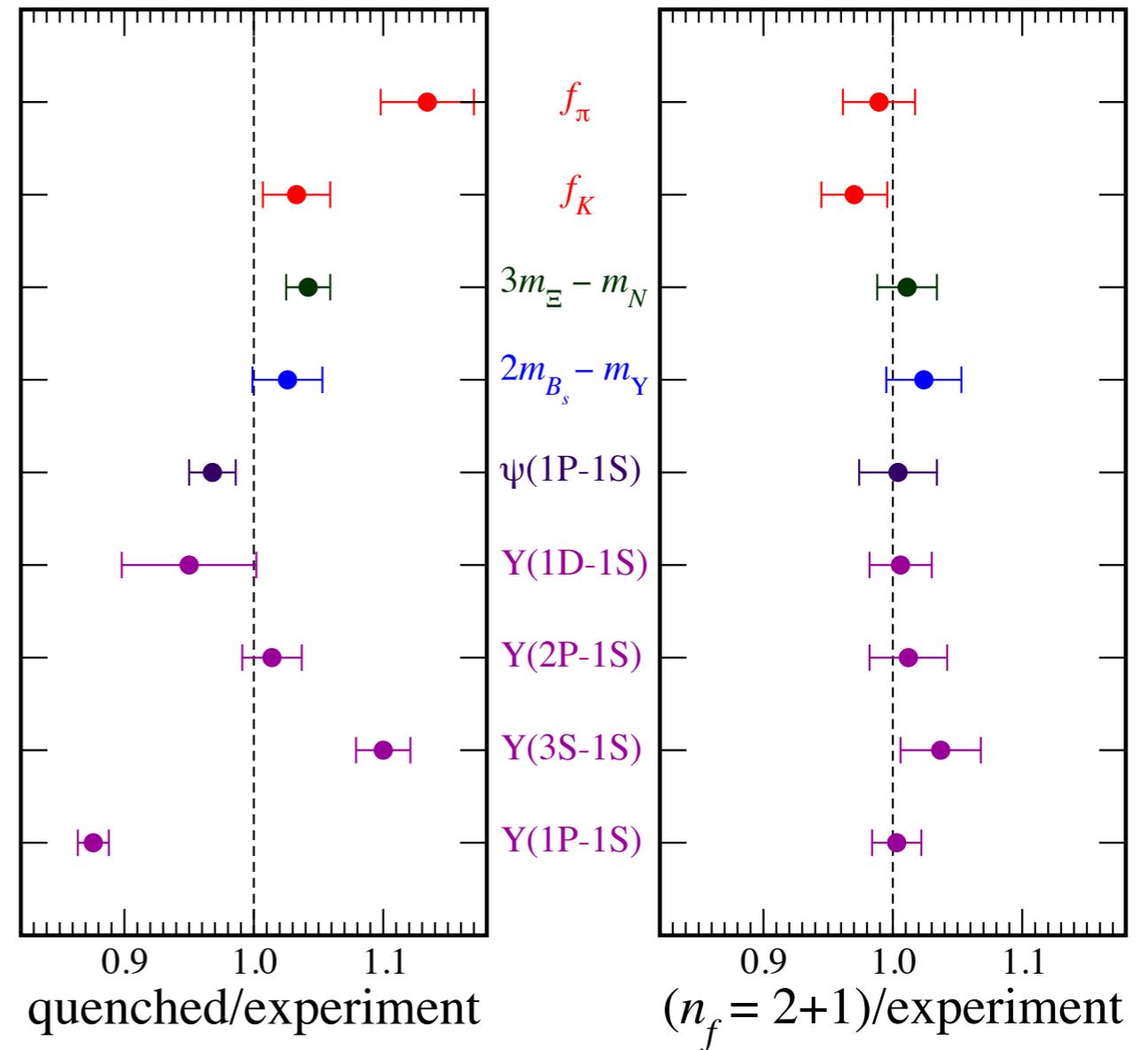
“Could you prepare half a dozen slides?  
Because John needs to give them to Mike,  
so Jim can show them to Pat.”

# High-Precision Lattice QCD Meets Experiment

# Lattice QCD Works!!!



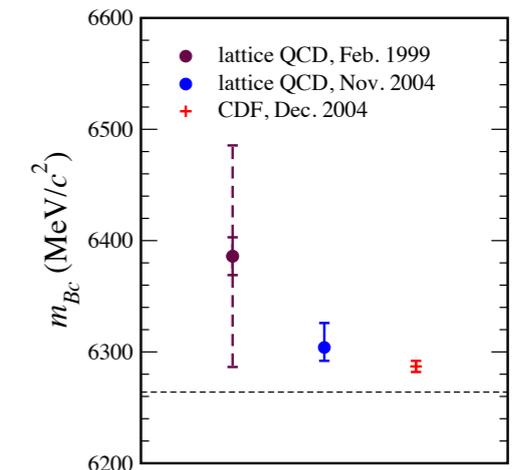
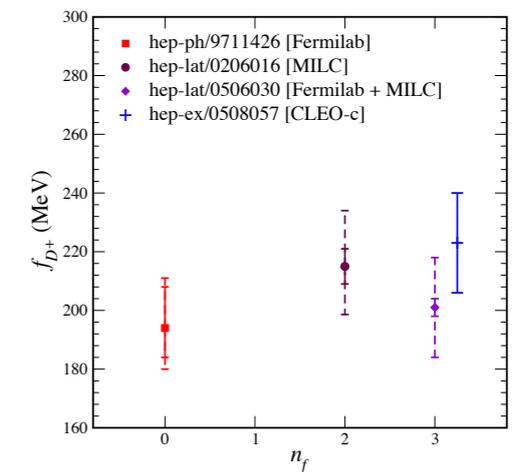
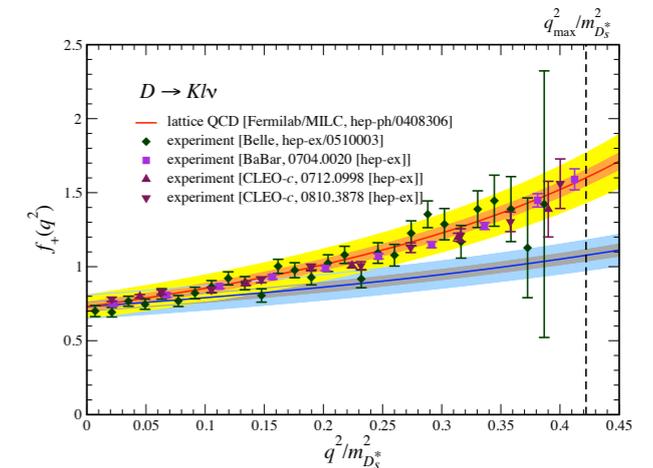
- MILC generated several ensembles with many good properties, esp. 2+1 sea quarks.
- Generously let others groups use them:
  - HPQCD
  - Fermilab Lattice
- Paul diplomatically brought us together for a landmark paper [[hep-lat/0304004](https://arxiv.org/abs/hep-lat/0304004)].



# Make Predictions



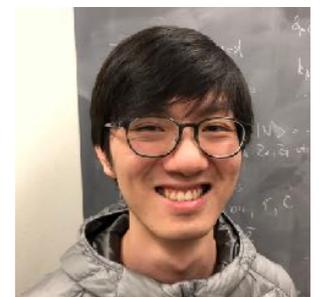
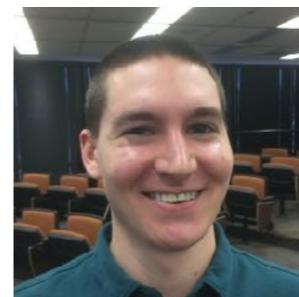
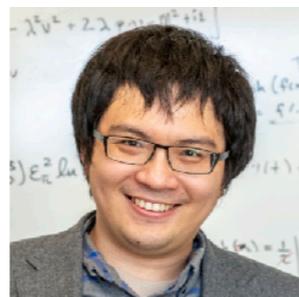
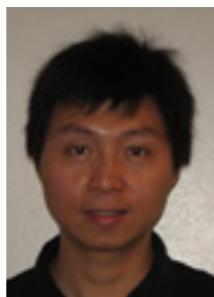
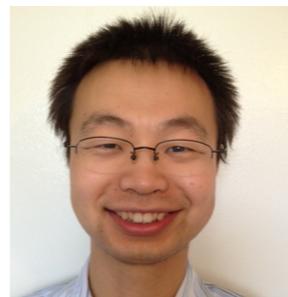
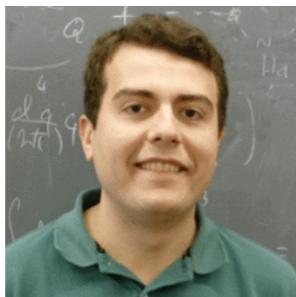
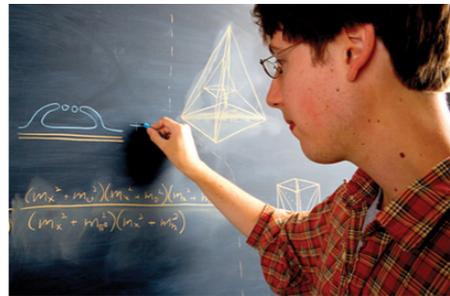
- Use the same ingredients to compute quantities that hadn't been (well) measured.
- Form factor in semileptonic  $D$ -meson decay [[hep-ph/0408306](#)].
- Leptonic decay constants of  $D_s^-$  &  $D$ -mesons [[hep-lat/0506030](#)].
- Mass of the  $B_c$  meson [[hep-lat/0411027](#)].



# CKM and Quark Masses Revisited

# Fuller Error Budgets

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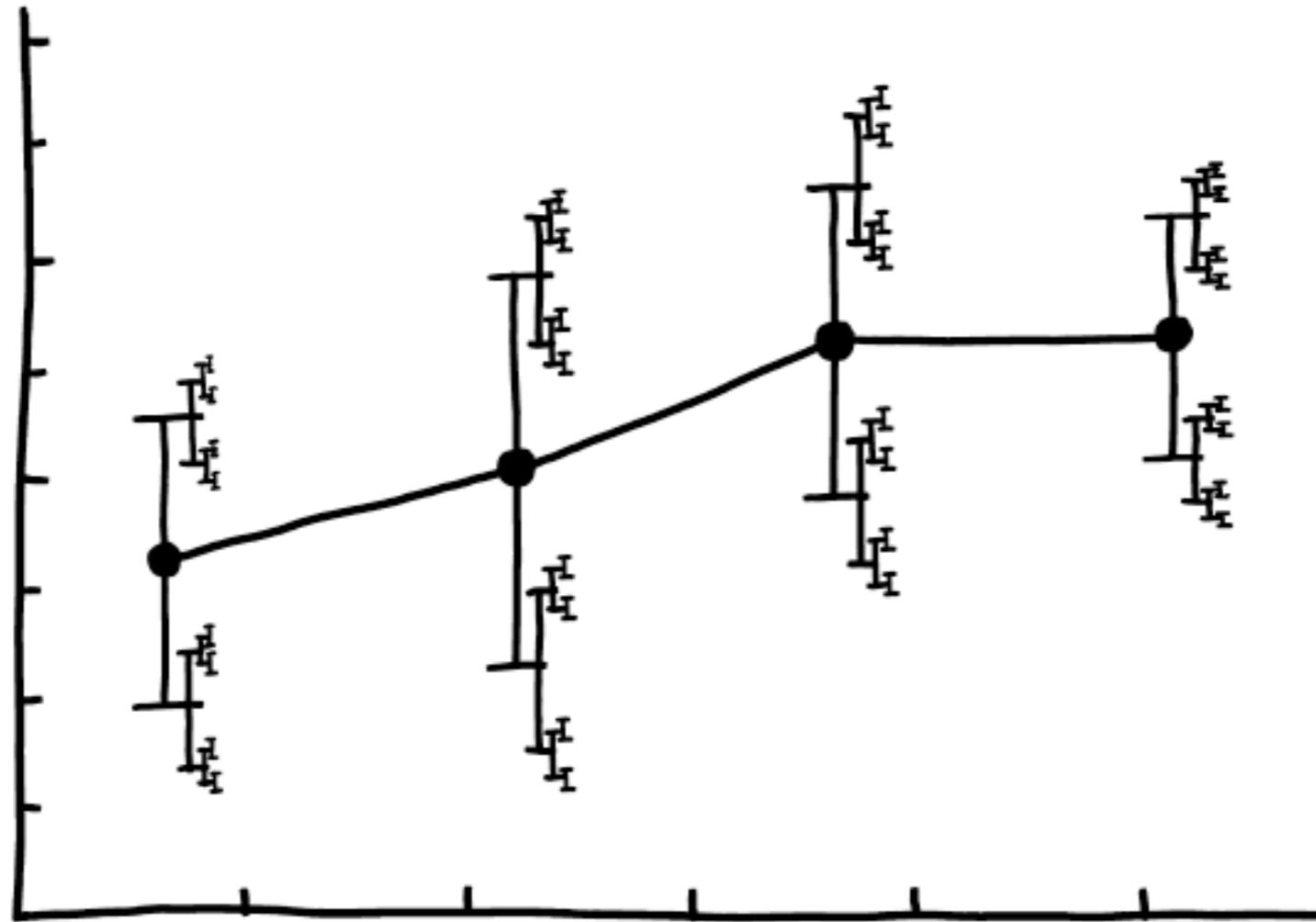
Closing Remarks

# The Real Lessons

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- Paul saw computation clearly albeit in a (sometimes) heterodox way.
- Some Mackenzian aphorisms:
  - "If an approximation breaks down somewhere, push it until it does break down, and see what the breakdown teaches you."
  - "Analyze all sources of uncertainty, including unimportant ones [they might matter next time] and impossible ones [otherwise your work is not so relevant]."
  - "The error bars have error bars!"
- Elements of the Fermilab "school", which Aida, Jim, and I also teach postdocs and students.

xkcd



I DON'T KNOW HOW TO PROPAGATE  
ERROR CORRECTLY, SO I JUST PUT  
ERROR BARS ON ALL MY ERROR BARS.



Thank you, Paul, for 30+ years of  
collaboration and friendship!